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We have employed spectral methods as well as direct simulations of the advection-diffusion equation to calculate the effective diffusivity for model flows. By calculating the eigenvalues and eigenvectors of a random matrix depending only on the fluid velocity field, we obtain the spectral measures used in Stieltjes integral representations for the effective diffusivity. The enhancement of thermal transport through sea ice by brine advection was also modeled using the advection-diffusion equation. Moreover, an inverse problem was formulated to study this enhancement of sea ice thermal conductivity and better understand temperature data collected during a 2007 Antarctic expedition.

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**ONR Grant N00014-12-10861:** Spectral Theory of Advective Diffusion in the Ocean


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Final Report

**Overview:** Mathematical models have been developed to investigate the effective transport properties of advective diffusion. In particular, we have employed spectral methods as well as direct simulations of the advection-diffusion equation to calculate the effective diffusivity for model flows. By calculating the eigenvalues and eigenvectors of a random matrix depending only on the fluid velocity field, we obtain the spectral measures used in Stieltjes integral representations for the effective diffusivity. The enhancement of thermal transport through sea ice by brine advection was also modeled using the advection-diffusion equation. Moreover, an inverse problem was formulated to study this enhancement of sea ice thermal conductivity and better understand temperature data collected during a 2007 Antarctic expedition.

**Activities and Findings:**

**1.** Advection-enhanced diffusion plays a central role in the transport of carbon, nutrients, salt, heat, and other climatically important tracers in the ocean. The advection-diffusion equation with a complex fluid velocity field is important to the study of such transport processes. The Golden-Papanicolaou formulation of the analytic continuation method was adapted by Avellaneda and Majda to the advection-diffusion equation for incompressible velocity fields, yielding a Stieltjes integral representation for the effective diffusivity tensor $\boldsymbol{\kappa}^*$, involving the Péclet number $Pe$ of the flow and a tensor valued spectral measure $\boldsymbol{\phi}$ of a random operator. However, explicit results are available only for simple flows, such as a shear flow.

To overcome this limitation we have adapted and extended the spectral method we developed for composite media, to directly calculate the spectral measure, hence the effective diffusivity, for complex velocity fields. In particular, we have been studying different regimes of advective diffusion for some model flows, such as shear flows, modified cat's eye flows, and vortical flows. A key feature of the method is that the calculations are not restricted to a specific range of Péclet numbers nor the complexity of the flow field. Our method provides a rigorous way of calculating the effective diffusivity for a large class of incompressible flows. Key results of this work include:

- *Functional analysis and the spectral theorem.* The mathematical framework underlying the Stieltjes integral representation for the effective diffusivity involves an abstract, infinite dimensional Hilbert space and a random operator which acts on the space. The spectral theorem of functional analysis, which provides the existence of the integral representation, depends critically on the properties of this Hilbert space. More specifically, it is only on a special subset of this space that the random operator is Hermitian, a required property for the existence of the integral representation. Translating this abstract framework to one for which numerical calculations can be made was a nontrivial task.

This task involved finding the appropriate random matrix which had the desired properties of the associated, infinite dimensional random operator on the Hilbert space. This analysis showed that the appropriate matrix is different from what was introduced in our proposal (but closely related), which is instead central to a variational formulation of the effective diffusivity. Once this task was accomplished, we adapted and extended spectral methods that we developed to study effective transport in composites, to study advection-enhanced diffusion by various incompressible fluid velocity fields, which are otherwise intractable by direct analytical calculation.

- *Matrix analysis, the projection method, and the effective diffusivity.* Once the appropriate random matrix described above was found, the corresponding spectral measure was explicitly calculated in terms of its eigenvalues and eigenvectors. This matrix is a composition of a symmetric projection matrix $\mathbf{\Gamma}$ and an antisymmetric matrix $\mathbf{H}$ which determines the fluid velocity field. In two dimensions, the matrix $\mathbf{H}$ is determined by a stream function $H(x,y)$. A careful analysis of the projective nature of $\mathbf{\Gamma}$ has revealed that the spectral measure depends only on the eigenvalues and eigenvectors of a much smaller Hermitian matrix. This projection method provides a computationally efficient way of calculating the spectral measure and the associated effective diffusivity by reducing the computational cost by a factor of eight. The diagonal components $\phi_{ii}$, $i=1,2$, of the spectral measure and the associated components $\kappa^*_{ii}$ of the effective diffusivity tensor for 2D shear and modified cat's eye flows are displayed in Figure 1 below, along with the theoretical prediction for shear flow: $\kappa^*_{11}/\kappa_0 = 1$ and $\kappa^*_{22}/\kappa_0 = 1 + Pe^2$, where $\kappa_0$ is the diffusivity of the fluid. This formula for $\kappa^*_{22}$ is an upper bound for $\kappa^*_{ii}$ over all flows with bounded Péclet number.

- *Numerical Efficiency and Stability.* The numerically efficient method for calculating the spectral measure described above has other important advantages. A numerical investigation has shown that this projection method significantly stabilizes the calculation as well. Stability in the calculation of an eigenvalue and its corresponding eigenvector is characterized in terms of the eigenvalue's *condition number.* A large condition number indicates that the calculation is unstable and prone to the propagation of round-off error. With our projection method, the condition number for the eigenvalue problem is reduced to order one from a more typical power of $N$, where $N$ is the grid size.

**2.** *Thermal transport through sea ice by brine advection.* The exchange of heat between the ocean and atmosphere through sea ice is a key process in the polar climate system. Thermal transport through sea ice can be enhanced when brine inclusions within the ice percolate at a volume fraction of $\approx 5\%$, giving fluid a connected pathway to flow through the entire thickness of the ice. To simulate this process, the advection-diffusion equation was used to model thermal transport through sea ice by brine advection.

Based on well-established theory, the effective Péclet number that characterizes the homogenized flow is proportional to the volume fraction of the brine inclusions. The enhancement of thermal conductivity, or more generally thermal diffusivity, through sea ice by brine advection can be estimated by temporal and spatial averaging of the heat flux across the ice boundaries, with air above and sea water below. We modeled the surface temperatures by time-periodic functions that mimic typical temporal variations. To simulate the enhancement of thermal transport through sea ice by brine advection, we performed

a sequence of computations with variations in the effective Péclet number of the homogenized flow. These variations are associated with brine volume fractions ranging from 5% (the onset of advection) to 12.5%. The enhancement of thermal conductivity due to brine advection through sea ice is displayed in Figure 2. Here, the shear flow is in the vertical direction, and the vortical flow consists of a periodic array of vortices perturbed slightly to resemble flows in actual sea ice. The difference in scales for the enhancement of the thermal conductivity between these two flows demonstrates the significance of the type of flow field.

**3.** *An inverse problem for thermal transport through sea ice.* Temperature measurements within sea ice are essential to modeling its effective thermal conductivity, and the usual approach is to form differences to estimate but this procedure can be affected by numerical instability and statistical noise. As an alternative to existing methodologies, we approached this from an inverse problem perspective.

We modeled a slab of sea ice by $n$ horizontal layers, with each layer represented by a fixed diffusivity value so that the diffusion equation can be easily solved. We used a nonlinear optimization algorithm to find the set of diffusivity values which leads to profiles that are closest to temperature profiles of data sets obtained by Jean-Louis Tison during a 2007 Antarctic expedition (SIMBA). We found that the most effective representation of the ice corresponds to a model of $n = 5$ layers, and the diffusivity of the bottom layer is significantly higher than the rest of the layers. The computed effective thermal conductivity values are substantially higher than that of the sea ice itself, in the absence of advection, at the same temperature and salinity. This indicates that the enhancement in thermal transport may be caused by brine advection. This is supported by adding a simple advection term to the model and finding the optimized diffusivity values closer to realistic values in sea ice, as well as better fits with the temperature profiles. In an ongoing effort, we are using an internal energy expression to separate conductivity information from the diffusivity, so that a direct comparison can be made with field data. We also plan to compare these results with rigorous bounds on the thermal conductivity that can be obtained from the Stieltjes representation. This work was done in collaboration with Daniel Liu, a high school student from West High School, Salt Lake City, UT.

**Expected Publications:**

N. B. Murphy, J. Zhu, and K. M. Golden, Spectral analysis of advective diffusion, preprint in preparation, to be submitted.

D. Liu, J. Zhu, J.-L. Tison, and K. M. Golden, Advection enhanced thermal transport in sea ice, preprint in preparation, to be submitted.

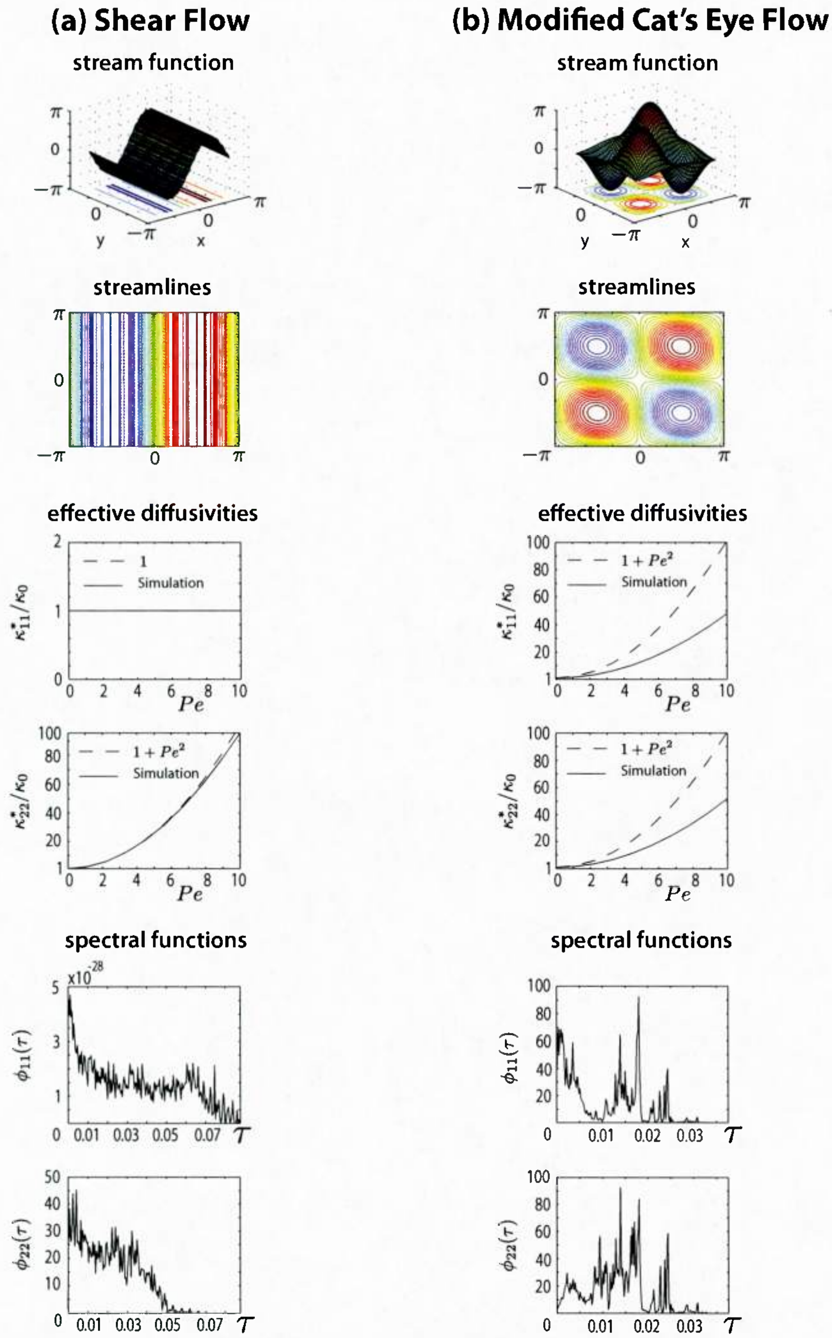


Figure 1: Effective diffusivities and spectral functions (histogram representations of the spectral measures) for model flows. The diagonal components of the effective diffusivity tensor $\kappa_{ii}^*$, $i = 1, 2$, and the spectral function $\phi_{ii}$ are displayed below the corresponding stream functions and streamlines. (a) Shear flow. The stream function is given by $H(x, y) = \sin x + (0.5 + \eta)\sin(15x)/15$ with $\eta$ uniformly distributed in the interval $(-0.1, 0.1)$. The theoretical prediction is $\kappa_{11}^*/\kappa_0 = 1$ and $\kappa_{22}^*/\kappa_0 = 1 + Pe^2$. (b) Modified cat's eye flow. The stream function is given by $H(x, y) = \sin x \sin y + \eta \cos x \cos y$.

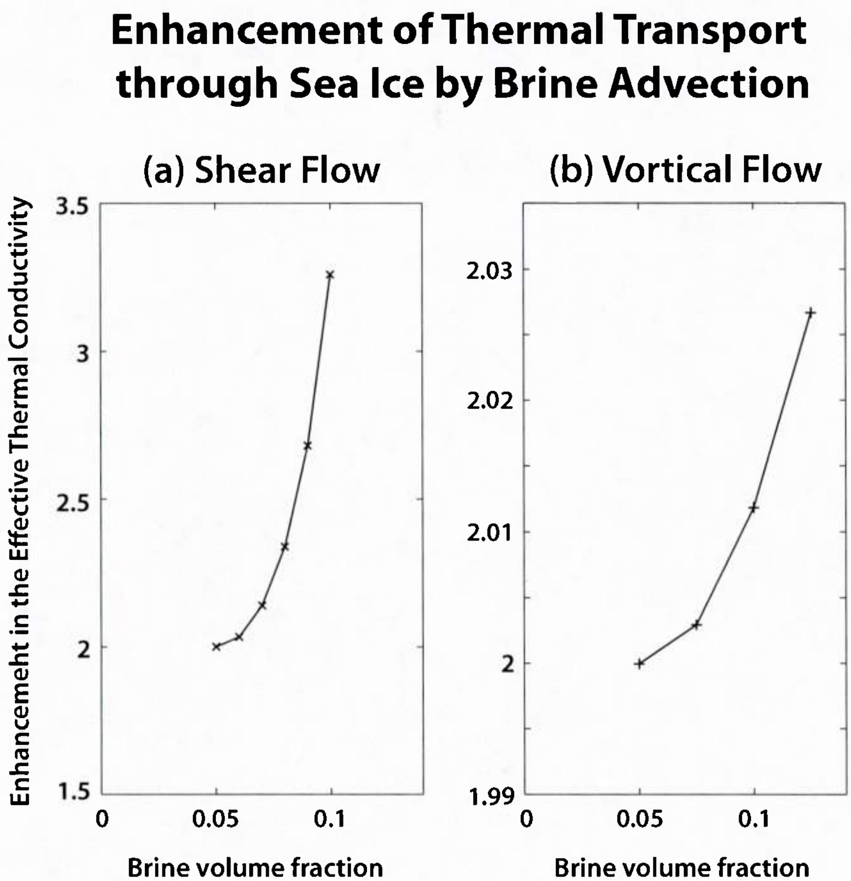


Figure 2: The enhancement of thermal conductivity of sea ice in the vertical direction due to brine advection. (a) The enhancement due to shear flow in the vertical direction. (b) The enhancement due to vortical flow (full matrix enhancement).